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14. ABSTRACT This grant was used to support the organization of the international conference "Multiscale Materials Modeling: Mathematical and Computational Aspects" at Rensselaer Polytechnic Institute, during the period June 10-12, 2014. The conference was organized under the auspices of the International Center for Applied Computational Mechanics (ICACM) and is the 8th meeting organized in this series. The conference brought together researchers from US, France and Canada working on various aspects of physics-based multiscale modeling of the mechanical behavior of materials. The details of the organization are presented in this report along with outcomes of the meeting relevant to the conference.					
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a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU			19b. TELEPHONE NUMBER 518-276-2195



## Report Title

Final Report: Mathematical and Computational Aspects of Multiscale Materials Modeling, Mathematics-Numerical analysis, Section II.A.a.3.4, Conference and symposia organization II.A.2.a

### ABSTRACT

This grant was used to support the organization of the international conference “Multiscale Materials Modeling: Mathematical and Computational Aspects” at Rensselaer Polytechnic Institute, during the period June 10-12, 2014. The conference was organized under the auspices of the International Center for Applied Computational Mechanics (ICACM) and is the 8th meeting organized in this series. The conference brought together researchers from US, France and Canada working on various aspects of physics-based multiscale modeling of the mechanical behavior of materials. The details of the organization are presented in this report along with outcomes of the meeting relevant for the future directions in this field.

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**Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:**

**(a) Papers published in peer-reviewed journals (N/A for none)**

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**TOTAL:**

**Number of Papers published in non peer-reviewed journals:**

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**(c) Presentations**

Number of Presentations: 0.00

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**Non Peer-Reviewed Conference Proceeding publications (other than abstracts):**

Received      Paper

**TOTAL:**

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

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**Peer-Reviewed Conference Proceeding publications (other than abstracts):**

Received      Paper

**TOTAL:**

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

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Received      Paper

**TOTAL:**

Number of Manuscripts:

Books

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TOTAL:

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TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

<u>NAME</u>	<u>PERCENT_SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT_SUPPORTED</u>
FTE Equivalent:	
Total Number:	

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### Names of Faculty Supported

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PERCENT SUPPORTED

**FTE Equivalent:**

**Total Number:**

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### Names of Under Graduate students supported

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This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: ..... 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

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Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

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### Names of Personnel receiving masters degrees

NAME

**Total Number:**

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### Names of personnel receiving PHDs

NAME

**Total Number:**

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### Names of other research staff

NAME

PERCENT SUPPORTED

**FTE Equivalent:**

**Total Number:**

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**Sub Contractors (DD882)**

## **Inventions (DD882)**

### **Scientific Progress**

The description of the activity is provided in the attached file.

### **Technology Transfer**

Report Type: Final Report  
Proposal Number: 64443MACF  
Agreement Number: W911NF1310203  
Proposal Title: Mathematical and Computational Aspects of Multiscale Materials Modeling, Mathematics-Numerical analysis, Section II.A.a.3.4, Conference and symposia organization II.A.2.a  
Report Period Begin Date: 09/16/2013  
Report Period End Date: 09/15/2014

## **Abstract**

This grant was used to support the organization of the international conference “Multiscale Materials Modeling: Mathematical and Computational Aspects” at Rensselaer Polytechnic Institute, during the period June 10-12, 2014. The conference was organized under the auspices of the International Center for Applied Computational Mechanics (ICACM) and is the 8<sup>th</sup> meeting organized in this series. The conference brought together researchers from US, France and Canada working on various aspects of physics-based multiscale modeling of the mechanical behavior of materials. The details of the organization are presented in this report along with outcomes of the meeting relevant for the future directions in this field.

## **Report**

### **Introduction**

The International Center for Applied Computational Mechanics was established 7 years ago by a group of researchers from France and US working in the field of Mathematics and Mechanics. The Center has organized meetings every year over the past 7 years.

The subjects covered in the past included, but were not limited to, geomaterials, energetic materials, plastic deformation in metals and alloys, granular materials etc. In all these meetings the focus was on mathematics, physics and computational aspects. Mathematical aspects included constitutive equations development, stability, stochasticity, uncertainty quantification, etc.

The conference has a simple format, with one common session. The talks are given only by invited speakers, while non-invited participants may present posters.

The meeting organized in 2014 (supported in part by this grant) continued along this path. The focus was on multiscale aspects of material behavior. This was the first meeting of the series having the mathematical, physical and computational integration of phenomena taking place on multiple scales as the central subject. Most previous meetings were focused on specific



scales, phenomena or material systems. Mathematical issues related to modeling, uncertainty quantification and error control were the central theme of the meeting.

**Previous meeting in this series were held at:**

2007: University of Florida, Shalimar  
2008: DGA, Rocamadour  
2009: University of Florida, Shalimar  
2010: University of Paris XIII, Institut Henri Poincaré  
2011: IUTAM Symposium, Florida  
2012: Rutgers University, New Jersey  
2013: University of Grenoble, France

**The goals of the meeting were:**

- Review the current state of modeling and understanding plastic deformation
  - Mathematical models
  - Computational techniques currently used
  - Multiscale modeling and multiscale experiments
  - Scale coupling
  - Role of instabilities
- Outline the outstanding challenges in both plasticity and multiscale modeling in general
- Promote interactions between participants

**Organization details:**

Speakers: 24

Registered participants, including invited speakers: 33

Actual number of participants, including local faculty, students and postdocs as well as visitors from General Electric, Research and Development: 45 to 50

Duration: 2 days

Length of talks: 30 or 40 minutes, 12 speakers per day

## Program:



ICACM 2014: Multiscale Materials Modeling: Mathematical and Computational Aspects

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### AGENDA, Tuesday, June 10, 2014

Room: Center for Industrial Innovation, CII 4050

8 :00            **Registration**

8 :20            **Welcome**

**Session 1.1** Chair: Catalin Picu

8 :30 – 9 :10    **Benoit Devincere**, CNRS-ONERA, The Discrete-Continuum Model: An Important Breakthrough to Simulate the Mechanical Properties of Dislocated Crystals with Complex Boundary Conditions

9 :10 – 9 :50    **Anter El-Azab**, Purdue University, Mathematical and Computational Modeling of Dislocation Patterns and Strain Hardening in Crystals

9 :50 – 10 :20   **Michael Demkowicz**, Massachusetts Institute of Technology, Interface Design Using Reduced Order Mesoscale Models

10 :20 – 10 :40   **Break**

**Session 1.2** Chair: Anter El-Azab

10 :40 – 11 :20   **James Sethna**, Cornell University, Bending Crystals: The Evolution of Cell Boundary Dislocation Structure

11 :20 – 11 :50   **Jianfeng Lu**, Duke University, Numerical Analysis of Atomistic-to-Continuum Hybrid Methods

11 :50 – 12 :20 : **Djimesdo Kondo**, Universite Pierre et Marie Curie Paris, Strength Properties of Ductile Nanoporous Materials: Theoretical Models and Assessment by Atomistic Simulations

12 :20 – 14 :00   **Lunch** – on site

**Session 1.3** Chair: Antoinette Maniatty

14 :00 – 14 :30   **Arash Yavari**, Georgia Institute of Technology, Non-Riemannian Geometries and the Nonlinear Mechanics of Distributed Defects

14 :30 – 15 :10   **David Srolovitz**, University of Pennsylvania, Atomistic Simulations of the Deformation of Nanocrystalline Metals: Applications to Dislocation Dynamics in Polycrystals

15 :10 – 15 :40   **Min Zhou**, Georgia Institute of Technology, Prediction of Macroscopic Fracture Toughness from Microstructure

15 :40 – 16 :00   **Break**

**Session 1.4** Chair: Min Zhou

16 :00 – 16 :30   **Nathan Barton**, Lawrence Livermore National Laboratory, Direct Multiscale Embedding of Polycrystal Plasticity Enabled by Adaptive Sampling

16 :30 – 17 :00   **Antoinette Maniatty**, Rensselaer Polytechnic Institute, Stabilized Finite Element Method for Multiscale Polycrystal Plasticity

17 :00 – 17 :30   **Regis Cottureau**, Ecole Centrale Paris, A Coupling Method for Stochastic Polycrystalline Models at Different Scales

19:00            **Dinner** (Russell Sage Dinning Hall, in campus)



## **AGENDA, Wednesday, June 11, 2014**

**Room: Center for Industrial Innovation, CII 4050**

### **Session 2.1** Chair: Ronald Miller

- 8 :30 – 9 :10 : **David McDowell**, Georgia Institute of Technology, Modeling Interface-Mediated Metal Plasticity at Small Scales
- 9 :10 – 9 :40 : **Ghiath Monnet**, RED R&D, MMC, Multiscale Simulations of Temperature and Strain Rate Sensitivity of Strengthening Induced by Coherent Precipitates: from Atomic to Continuum Scale
- 9 :40 – 10 :10 : **David Rodney**, Universite de Lyon, Overcoming Old Barriers in Thermally-Activated Plasticity
- 10 :10 – 10 :30 : **Break**

### **Session 2.2** Chair: David Rodney

- 10 :30 – 11 :00 : **Ronald Miller**, Carleton University, Finite Temperature and Finite Deformation: New Tools for More Efficient and Accurate Atomistic Simulation
- 11 :00 – 11 :40 : **Armand Beaudoin**, University of Illinois at Urbana-Champaign, Study of Microplasticity Through 3D X-ray Diffraction
- 11 :40 – 12 :20 : **Michel Potier-Ferry**, Universite de Lorraine, Multi-scale Instabilities
- 12 :20 – 14 :00 : **Lunch** – on site

### **Session 2.3** Chair: Ioan Ionescu

- 14 :00 – 14 :30 : **Jerome Weiss**, Universite Joseph Fourier Grenoble, From Continuous to Crackling Plasticity
- 14 :30 – 15 :00 : **Hamed Hatami-Marbini**, Oklahoma State University, An Experimental and Computational Framework for Investigating the Mechanical Behavior of Corneal Stroma
- 15 :00 – 15 :40 : **Jacob Fish**, Columbia University, Practical Multiscaling
- 15 :40 – 16 :00 : **Break**

### **Session 2.4** Chair: Jerome Weiss

- 16 :00 – 16 :40 : **Jia Li**, Universite de Paris Nord, Interaction Between Anisotropic Damage and Dynamic Wave Propagation in Brittle Materials
- 16 :40 – 17 :10 : **Vivek Shenoy**, University of Pennsylvania, Multiscale Modeling of Compositional Stresses in Nonstoichiometric Oxides
- 17 :10 – 17 :40 : **Assad Oberai**, Rensselaer Polytechnic Institute, Subgrid Models for Multi-Parameter Problems

18:00 **Departure to Saratoga Springs for dinner**

## **Outcomes of the meeting: Outstanding research issues identified by the participants**

- The representations of dislocations on various scales are entirely different (explicit atomistic models, discrete dislocation dynamics models (DDD), continuum representations). Coupling of these models is difficult. Coupling of atomistics and DDD models has been explored to some extent, but the coupling between DDD and continuum models of the evolution of large populations of dislocations is essentially unexplored.

None of these models account for additional complexities introduced for example by the presence of solute, precipitates and twins.

- In particle models, coarse grained representations have been developed using rather formal methods (e.g. Mori-Zwanzig). This formulation allows writing the evolution equation for the coarse system (or the associated Liouvillian). From this, it is possible to go further to larger scales to develop DPD (dissipative particle dynamics) or even fluid mechanics models. In the case of plastic deformation and associated fracture and damage accumulation, no such coarse graining methodology has been developed so far. This is one of the important missing links in multiscale modeling of material behavior.

- Concurrent coupling of models of the Quasicontinuum type are still to be developed, especially at non-zero temperatures. There are big computational challenges in 3D and simply using larger computers is not a solution.

- An emergent view of plastic deformation is that of a non-monotonic process, which takes place by large jumps forward separated by periods when there seems to be little activity. These have been termed “avalanches” and are different from larger scale instabilities. Avalanches have been observed on the small scales in many material systems, mainly by acoustic emission experiments. Although the deformation is unsteady on the small scales (microns and below), it appears steady on larger scales. The “smoothing” out of this process is not properly represented in any current models of deformation.

The relationship between plastic deformation and critical phenomena is currently being explored.

- The use of non-Riemannian geometry to represented bodies with defects is still being explored. The concept here is that one can map the real space in which materials carry residual stresses to a curved space in which the equivalent configuration is stress-free. This presents the advantage that as one applies deformation, the initial state is well-defined and a real reference configuration. In addition, the deformation itself can be defined as an evolution of the mapping bringing the system from real space to the fictitious described above. This method has is similar to that used in relativity to account for space curvature, but its application to mechanics of classical continua has not been explored extensively in the recent years.

- In many situations one needs to compute energetic barriers for various processes. This is usually done using transition state methods, such as the Nudged elastic band method. These methods provide the path taken by the system in phase space as it evolves between two

equilibrium configurations. The point of highest energy on this path is the energetic barrier of interest. Many methods that address this problem exist. However, none of these is perfect. Improvements in this area are very much needed.

- The validity of interatomic potentials used in atomistic models of matter is an important, recognized issue. Potentials provide only approximations of the real interactions and are bound to fail in regions where large strains and strain gradients exist (e.g. at defect cores). Efforts are continuously made to improve potentials. This problem is conceptually identical to the error introduced in larger scale models due to coarse graining steps taken on sub-scales. There is no simple, theoretical answer for this issue.
- Uncertainty propagation. The mathematical issue of how uncertainty propagates across scales and from one model to another is of great importance. A related issue is to ask: how variability (moments larger than one of the distribution function) of fields influences the mean (first moment of the distribution function) of the system scale response.